A computationally efficient Q-tensor model with flow for nematic liquid crystals

Y. Murugesan(1), G. De Matteis(2) and G. D’Alessandro(1)∗

1 Mathematical Sciences, University of Southampton, Southampton, England, UK
2 Department of Mathematics and Information Sciences, Northumbria University, Newcastle Upon Tyne, England, UK

We present a new, computationally efficient method to model the flow and alignment of nematic liquid crystals in the absence of defects.

Traditionally, there are two approaches to model liquid crystal alignment with flow. In the Ericksen-Leslie formalism[1,2] the director field is represented with a unit vector $\mathbf{n}$ and the alignment dynamics of the director is coupled to the velocity field of the fluid flow. Sonnet et al[3] represent the director field using a $3 \times 3$ traceless, symmetric tensor, the $Q$-tensor, and obtain the alignment and fluid flow equations from the most generic dissipation function that satisfies the symmetries of the system.

From a computational point of view the two approaches have both pros and cons. The equations for the vector representation have only one time constant and are, hence, computationally efficient. On the other hand, they suffer from the ambiguity (nematic symmetry) that $\mathbf{n}$ and $-\mathbf{n}$ represent the same director. The $Q$-tensor representation, instead, can represent without ambiguity any alignment and embodies the nematic symmetry automatically. Moreover, it takes into account the orientational order of the liquid crystal by including the thermotropic energy in addition to the elastic counterpart. On the other hand, due to the two energy contributions, the corresponding dynamical equations for the director alignment have two considerably different time scales: the resulting computational model is, hence, very stiff and hard to compute efficiently.

To overcome the stiffness of the $Q$-tensor representation, while preserving its ability to represent any nematic liquid crystal alignment, we have developed an approximate theory[4] to model the director field alignment in the absence of fluid flow. This approximation is based on the observation that the two time scales of the $Q$-tensor dynamics correspond to two physical phenomena. In the absence of defects, the $Q$-tensor dynamics relaxes very rapidly to a disordered nematic state, represented mathematically by an invariant manifold. The slow time scale represents the alignment of the liquid crystal under the influence of elastic forces and external fields. Mathematically this is represented by a trajectory tangent to the invariant manifold. Using the method of multiple scales it is possible to write separately the equations for the motion tangent to the manifold, i.e. it is possible to obtain a computationally efficient, one-time-scale $Q$-tensor model in the absence of defects.

In this paper we extend this approach to include fluid flow: we combine the $Q$-tensor with flow equations of Sonnet et al[3] with the multiple scale approach developed by Daly et al[4] and obtain a one time constant set of equations for the alignment of the liquid crystal coupled with fluid motion. As a check of our derivation we compare our results with the Ericksen-Leslie theory for 1D planar cells and discuss the differences between these two approaches.

References:

∗Presenting author, E-mail: dales@soton.ac.uk